

1,3-Naphthalenediol
132-86-5 | DTXSID8059631

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.01e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.11e-01

Confidence level: 5.93e-01

Nearest Neighbors from the Training Set

Image not found

1,5-Dihydroxynaphthalene

Measured: 1.03e-03

Predicted: 8.87e-03

Image not found

1,3-Naphthalenediol

Measured: 1.12e-02

Predicted: 2.01e-02

Image not found

2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 1.45e-01

Predicted: 2.34e-01

Image not found

Tribromoacetic acid

Measured: 6.74e-01

Predicted: 5.34e-01